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Thermophysics Characterization of Kerosene Combustion

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A one-formula surrogate fuel formulation and its quasi-global combustion kinetics model are developed to support the design of injectors and thrust chambers of kerosene-fueled rocket engines. This surrogate fuel model depicts a fuel blend that properly represents the general physical and chemical properties of kerosene. The accompanying gaseous-phase thermodynamics of the surrogate fuel is anchored with the heat of formation of kerosene and verified by comparing a series of one-dimensional rocket thrust chamber calculations. The quasi-global combustion kinetics model consists of several global steps for parent fuel decomposition, soot formation, and soot oxidation and a detailed wet-CO mechanism to complete the combustion process. The final thermophysics formulations are incorporated with a computational fluid dynamics model for prediction of the combustion efficiency of an unelement, tripropellant combustor and the radiation of a kerosene-fueled thruster plume. The model predictions agreed reasonably well with those of the tests.

Nomenclature

| | | |
|----------|---|--|
| A | = | preexponential factor, $(\text{mol}/\text{cm}^3)^{1-n} \text{K}^{-B}/\text{s}$ |
| B | = | temperature power dependency |
| C_p | = | heat capacity, cal/mol-K |
| D | = | diameter, cm |
| E | = | activation energy, cal/mol |
| H | = | enthalpy, cal/mol |
| K | = | forward rate constant, $(\text{mol}/\text{cm}^3)^{1-n}/\text{s}$ |
| n | = | order of reaction |
| P | = | pressure, atm |
| Q | = | radiative heat flux, Btu/ft ² -s |
| R | = | universal gas constant, cal/mol-K |
| S | = | entropy, cal/mol-K |
| T | = | temperature, K |
| α | = | species mass fraction |
| θ | = | view angle, deg |
| ρ | = | density, g/cm ³ |

Subscripts

| | | |
|-----|---|-----------------------|
| c | = | combustion or chamber |
| f | = | formation |
| s | = | soot |

Introduction

RUSSIAN-BUILT kerosene-fueled rocket engines such as RD-170 (Ref. 1) or its U.S. proposed counterparts such as RD-704, Fastrac engine, and rocket-based combined-cycle hydrocarbon engine have been identified as potential candidates to fly the single-stage-to-orbit reusable launch vehicles. To support the associated engineering issues, specifically the preliminary conceptual design and evaluation of the performance of the injectors and thrust chambers using computational fluid dynamics (CFD), accurate and computationally efficient models that properly represent the thermophysics, namely, fuel formula, thermodynamics, and finite-rate combustion kinetics, have to be used. Unfortunately, models pertaining to these aspects were underdeveloped.

In this study, based on reported thermophysical–chemical property data, a one-formula surrogate fuel is proposed as a generic repre-

sentation for kerosene or its derived fuel, rocket propulsion (RP)-1. The thermodynamics of the surrogate fuel such as heat capacity, enthalpy, and entropy are generated, and the rationale for generation is given. Kerosene combustion kinetics is proposed based on a quasi-global kinetics format, and the rationale for it, including the specific reactions chosen, is also given. The final thermophysics characterization is implemented in a CFD model and benchmarked on two rocket applications: the combustion efficiency of an experimental tripropellant combustor and the radiation of a test rocket plume.

One-Formula Surrogate Fuel Model

Common hydrocarbon rocket fuels such as kerosene or jet fuels are derived from petroleum, whereas RP-1 is a straight run kerosene fraction.^{2,3} These hydrocarbon fuels are complex mixtures of many components, and their exact composition and properties vary from batch to batch. Some information on these substances has been reported in the literature. For example, it is reported⁴ that kerosene typically consists of 10 hydrocarbons containing 10–16 carbon atoms per molecule, whereas the constituents include *n*-dodecane, alkyl derivatives of benzene, and naphthalene and its derivatives. Also, at least 87 identifiable hydrocarbons are reported in RP-1 (Ref. 5).

It is obvious that using all 87 identifiable hydrocarbons to represent RP-1, or even 10 species for kerosene would be highly inefficient in any kind of performance calculations. A surrogate fuel model composed of a neat compound or several neat components for kerosene-derived fuels has to be developed, while important thermophysical properties such as the heat of combustion are retained. Such a simplification is necessary for computation-intensive design calculations using complex fuels or blends. Conventionally, elemental formulas such as $\text{CH}_{1.9423}$ and its derived standard heat of formation have been used in one-dimensional theoretical rocket performance calculations⁶ for jet propulsion (JP)-4 and RP-1 powered engines. However, elemental formulas have severe limitations when design calculations other than one-dimensional performance is desired, especially those using CFD codes where molecular fuel formulas are preferred. In the past, several nonelemental one-formula surrogate fuel models were proposed. For example, one-formula models $\text{C}_{10}\text{H}_{19}$ (Ref. 7) and $\text{C}_{12}\text{H}_{23}$ (Ref. 4) were used to represent kerosene, whereas $\text{C}_{12}\text{H}_{26}$ (Refs. 8 and 9) was used to replace RP-1. The simplistic nature of those one-formula fuel models makes them easy to use. However, those simple formulas present subtle problems when used in performance calculations. For example, when compared to the physical–chemical properties of kerosene and RP-1, the molecular weight of $\text{C}_{10}\text{H}_{19}$ is too low, the H/C ratio of $\text{C}_{12}\text{H}_{23}$ is too low, and the H/C ratio of $\text{C}_{12}\text{H}_{26}$ is too high. Furthermore, $\text{C}_{12}\text{H}_{26}$ (*n*-dodecane) is paraffin whereas kerosene normally contains only 41% noncyclic hydrocarbons.

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Table 1 Comparison of thermophysical-chemical characterization of model fuel with reported data

| Property | Kerosene | RP-1 | Surrogate fuel |
|---|------------------|--|---|
| Molecular formula | — | — | C ₁₂ H ₂₄ |
| Molecular weight | 175 (Ref. 10) | 172–175 (Ref. 2) | 168 |
| Elemental formula | — | CH _{1.95} –CH _{2.0} (Ref. 2) | CH _{2.0} |
| Formula weight | — | CH _{1.9423} (Ref. 6), CH _{1.953} (Ref. 10) | 14.03 |
| H _c , kcal/g | –10.278 (Ref. 3) | 13.97–14.03 (Ref. 3), 13.97 (Ref. 6) | –10.278 |
| | –10.321 (Ref. 7) | –10.241 (Ref. 2) | |
| | | –10.356 (Ref. 6) | |
| H _{f,298K} , kcal/mole | — | –5.430 (Ref. 6)/CH _{1.9423} | –92.200/C ₁₂ H ₂₄ , –7.683/CH _{2.0} |
| C _{p,516k,1atm} cal/mole · K | — | 101 (Ref. 2) | 103 |
| Paraffins (<i>n</i> and <i>iso</i>) % | — | 41 (Ref. 2) | 41.7 |
| Naphthenes, % | — | 56 (Ref. 2) | 58.3 |
| Aromatics, % | 5 (Ref. 3) | 5 (Ref. 11), 3 (Ref. 2) | 0 |
| Olefins, % | 1 (Ref. 3) | 0 (Ref. 2) | 0 |

Other than the elemental formula and one-formula fuel models, a more detailed modeling approach is the multiple-formula models. For example, Farmer and Anderson⁵ used a three-formula surrogate fuel model to represent RP-1, that is, 17.4% C₁₃H₁₂ (methylbiphenyl), 45.4% C₁₂H₂₄ (*n*-heptylcyclopentane), and 37.2% C₁₂H₂₈ (*n*-tridecane). With multiple molecules, the physical-chemical properties of kerosene or RP-1 may be matched better. However, this approach often creates extra chemical species, thereby slowing down the computation. After weighing the advantages and disadvantages of the one-formula and multiple-formula approaches, a one-formula surrogate fuel C₁₂H₂₄ is proposed as a generic representation for kerosene or RP-1. Because only one parent fuel is involved, there is computational efficiency. In addition, although C₁₂H₂₄ takes the form of a one-formula surrogate fuel, it is modeled (kinetically) as 41.7% paraffin and 58.7% naphthene, matching approximately the reported paraffin/naphthene split^{2,3} of $\frac{41}{56}$. In fact, C₁₂H₂₄ does not represent a certain molecule, but rather a mixture of many neat components that have the same averaged thermophysical-chemical characterization as that of the reported kerosene/RP-1. Therefore, C₁₂H₂₄ has the advantages of a multiple-formula surrogate fuel without being represented as multiple fuels. In summary, the (averaged) molecular weight, elemental formula and formula weight, and the paraffin/naphthene split of the surrogate fuel C₁₂H₂₄ match reasonably well with those of kerosene and RP-1 (see Table 1 and Refs. 2, 3, 6, 7, 10, and 11). The paraffin-to-naphthene split is an important factor to match in terms of accurate soot prediction because soot forms much easier from naphthene than from paraffin. This point will be elaborated in the quasi-global combustion kinetics section. Notice the small amount of aromatics and olefins in kerosene and RP-1 lumped into the paraffins and naphthenes of the surrogate fuel model.

Gaseous-Phase Surrogate Fuel Thermodynamics Generation

An important thermodynamic property to be considered for the surrogate fuel is the heat of formation if accurate heat release during combustion is to be predicted. In general, the heat of formation cannot be measured directly but must be determined indirectly from its heat of combustion, which is measured calorimetrically. The heat of formation for the surrogate fuel is therefore determined by matching its heat of combustion with that of kerosene/RP-1. This is accomplished by writing a complete combustion reaction for C₁₂H₂₄:



The heat of reaction of this equation is the heat of combustion. By definition, the net heat of combustion is obtained when the product H₂O is at its gaseous state. The heat of formation of the surrogate fuel is written as

$$H_{f,\text{C}_{12}\text{H}_{24}} = 12H_{f,\text{CO}_2} + 12H_{f,\text{H}_2\text{O}} - H_c$$

The preceding equation underscores the importance of an appropriate fuel model because the stoichiometry of the combustion reaction determines the value of the molar heat of formation and eventually

Table 2 Thermodynamic coefficients for C₁₂H₂₄

| Coefficient | 1000–5000 K | 300–1000 K |
|-----------------------|-----------------|-----------------|
| <i>a</i> ₁ | 0.36440206E+02 | 0.39508691E+01 |
| <i>a</i> ₂ | 0.54614801E–01 | 0.10207987E+00 |
| <i>a</i> ₃ | –0.16091151E–04 | 0.13124466E–04 |
| <i>a</i> ₄ | 0.21478497E–08 | –0.76649284E–07 |
| <i>a</i> ₅ | –0.10131180E–12 | 0.34503763E–10 |
| <i>a</i> ₆ | –0.63890109E+05 | –0.52093574E+05 |
| <i>a</i> ₇ | –0.15798973E+03 | 0.21980951E+02 |

the amount of combustion products in the engine system. Several reported standard heats of combustion are listed in Table 1. The maximum difference among them is only 0.115 kcal/g and amounts to about 1% of the heating value. These values are deemed as consistent and are within the uncertainty bound of the measurement. A midrange value of –10.278 kcal/g is chosen. As a result, a thermodynamically consistent heat of formation of –92.200 kcal/mole is derived for C₁₂H₂₄, and a value of –7.683 kcal/mole is calculated for its elemental form CH_{2.0}, as shown in Table 1.

The next step is to construct the three thermodynamic functions of heat capacity, enthalpy, and entropy as functions of temperature in a usable form. The standard fourth-order polynomial heat capacity form⁶ is used:

$$C_p/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$H/RT = a_1 + (a_2/2)T + (a_3/3)T^2 + (a_4/4)T^3 + (a_5/5)T^4 + (a_6/T)$$

$$S/R = a_1 \ln T + a_2T + (a_3/2)T^2 + (a_4/3)T^3 + (a_5/4)T^4 + a_7$$

The enthalpy of the surrogate fuel is constructed using the heat capacities of *n*-dodecane, due to the closeness of *n*-dodecane (C₁₂H₂₆) with the C₁₂H₂₄ family of molecules in terms of carbon and hydrogen atomic numbers and the notion^{4,5} that *n*-dodecane is a major component in kerosene/RP-1. Notice the enthalpy (heat) of formation is anchored with the thermodynamically consistent heat of combustion of kerosene/RP-1. Hence, the generated heating curve is more realistic than that of Ref. 4 in which the enthalpy of *n*-dodecane was used as a placeholder. The generated heat capacity for the surrogate fuel matches well with that of RP-1, as indicated in Table 1. The entropy of formation of *n*-dodecane is used to construct the entropy curve for C₁₂H₂₄. The resulting least-square coefficients fitted for two temperature ranges are listed in Table 2.

Notice that the reported² magnitude of the heat of vaporization of kerosene (0.059 kcal/g at normal boiling point) is not only much smaller than that of the heat of combustion, but is also less than the error bound (0.115 kcal/g) (Refs. 2, 3, 6, and 7). In addition, the latent heat decreases to zero at critical pressure because most of the rocket engines are operated at higher pressures. These rationales allow the gaseous-phase thermodynamics to be curve fitted to 300 K, about 242 K lower than the normal boiling point (542 K) (Ref. 2) of kerosene. Nevertheless, in actual calculations involving liquid

kerosene fuel, the heat capacity and latent heat of vaporization of liquid kerosene¹² are used for the liquid-phase thermodynamics, as shown in latter sections of this study. A continuous thermodynamics model¹³ is an alternative for multicomponent droplet vaporization calculations.

Surrogate Fuel Thermodynamics Validation

From a thermochemical consistency standpoint, the proposed one-formula surrogate fuel and its thermodynamic coefficients can be validated by performing a series of one-dimensional theoretical rocket engine performance calculations, by use of the thrust chamber specifications and operating conditions of a Russian engine RD-170 (Refs. 1 and 10). Figure 1 shows a comparison of the calculated theoretical chamber and nozzle exit temperatures as a function of mixture ratios for $C_{12}H_{24}$ and its elemental formula $CH_{2,000}$ for the self-consistency test. Notice the thermodynamic coefficients are used for $C_{12}H_{24}$ and the heat of formation is used for $CH_{2,000}$. The calculated temperatures for $C_{12}H_{24}$ and $CH_{2,000}$ coincide, as expected, because their heat of formations are anchored with the chosen heat of combustion at -10.278 kcal/g. Also shown in Fig. 1 are the results using elemental formula $CH_{1,9423}$ with heats of formation of -5.430 , -6.613 , and -7.133 kcal/mole. These values correspond to heats of combustion of -10.356 (Ref. 6), -10.278 (Ref. 3), and -10.241 (Ref. 2) kcal/g, respectively. The difference among the curves is small because the difference in heats of combustion is small, especially in the fuel lean region. When the temperature profiles are compared at the same heat of combustion (-10.278 kcal/g), the minor difference between CH_2 and $CH_{1,9423}$ curves is the result of their difference in H/C ratios.

Figure 2 shows the predicted theoretical nozzle exit gas composition. Again, the species mole fractions resulted from using $C_{12}H_{24}$

coincide with those of $CH_{2,000}$. Graphite carbon C, and methane gas form at low mixture ratios due to fuel-rich combustion at low temperatures, as expected. These results show that the proposed one-formula surrogate fuel model is suitable for one-dimensional theoretical rocket performance calculations and is thermodynamically consistent. However, note that the system type of calculations often overpredicts the performance, especially for heavy hydrocarbon-fueled engines. This is because performance impacting thermophysical processes such as the finite-rate chemistry, ignition delay times, and vaporization are not considered. In addition, other performance impacting and design particular physical processes such as mixing, shock losses, geometry losses, film cooling, and boundary-layer losses are also not included.

Quasi-Global Finite-Rate Combustion Kinetics

Kerosene Decomposition and Wet-CO Mechanism

Detailed kinetics mechanism involving elementary steps for parent fuel decomposition is computationally prohibitive for considering kerosene/RP-1 combustion in CFD calculations. On the other hand, one-step⁴ and multiple-step global kinetics models¹⁴ are computationally efficient, but frequently overpredict the flame temperature, or are not generic enough to take advantage of the modern diagnostic techniques. For example, hydroxyl radical (OH) is usually not involved in those models and so laser-induced fluorescence imaging of the OH-radical flame structure data¹⁵ cannot be utilized. The quasi-global kinetics that combines several global steps with a detailed wet-CO mechanism is probably best suited for describing complex fuel combustion in a computationally intensive environment. The original quasi-global kinetics¹⁶ was established based on the observation that straight-chain hydrocarbons and cyclic hydrocarbons have distinctively different ignition delay time characteristics and that the ignition delay times for straight-chain hydrocarbons are similar and so are those for cyclic hydrocarbons. That important observation led to the development of the original quasi-global kinetics model in which two irreversible global steps are used to describe the decompositions of the straight-chain hydrocarbons and the cyclic hydrocarbons, respectively, and a detailed wet-CO mechanism converts the intermediates into the final combustion products. In the quasi-global kinetics format, OH radical is not only considered (in the wet-CO mechanism), but plays a vital role in the accurate prediction of the heat release. The original quasi-global kinetics scheme¹⁶ was evaluated with a variety of simplified flow configurations, including the stirred reactors, plug flow reactors, and turbulent diffusion flames. It was later expanded to an extended quasi-global kinetics model^{17,18} in which two more intermediate species and several more global kinetic steps are added to better describe the fuel-rich combustion. In this study, under the premises of computational efficiency and the framework of one-formula surrogate fuel model, the original quasi-global kinetics format is considered. Following that format, two global steps are proposed: one for the paraffin portion and another for the naphthene part of the surrogate fuel. The rates of the two global steps are modified directly from those of the straight-chain and cyclic global steps¹⁶ according to the paraffin and naphthene split in the proposed surrogate fuel ($C_{12}H_{24}$), thereby satisfying the ignition delay times requirement of the original quasi-global kinetics model. The proposed kerosene global steps and the existing CO-wet mechanism are shown in Table 3. The standard form in the fourth column of Table 3 means the species concentration terms in the rate expression follows the stoichiometry of the reaction. The forward reaction rate constant is expressed in the standard Arrhenius form. The backward reaction rate of the reversible reaction is calculated from its forward rate and the equilibrium constant.

Soot Formation

Under fuel-rich conditions, kerosene/RP-1 forms soot readily. This is because naphthene and aromatic hydrocarbons form soot rapidly (condensation-polymerization) by directly condensing themselves into polycyclic aromatic hydrocarbons (PAH), also known as the soot precursors. On the other hand, paraffins form

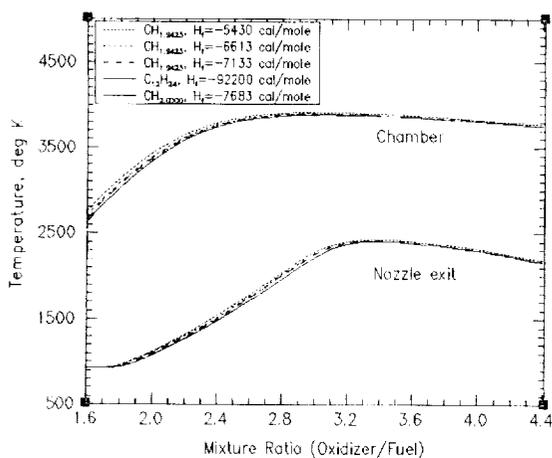


Fig. 1 Comparison of the RD-170 chamber and nozzle exit temperatures.

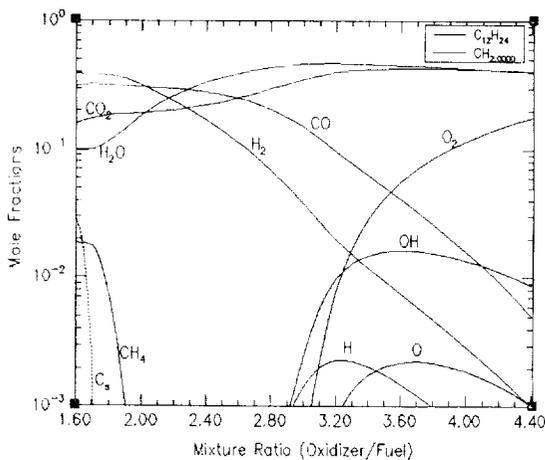


Fig. 2 RD-170 nozzle exit gas composition.

Table 3 Kerosene/RP-1 quasi-global combustion kinetics mechanism

| Reaction ^a | A | B | E/R | Form | Ref. |
|---|-----------|-------|----------|-------------------------------------|-----------------|
| <i>Paraffin global step</i> | | | | | |
| $C_{12}H_{24} + 6O_2 \rightarrow 12CO + 12H_2$ | 3.888E4 | 1 | 1.220E4 | $p^{0.3}[C_{12}H_{24}]^{0.5}[O_2]$ | This work |
| <i>Naphthene global step</i> | | | | | |
| $C_{12}H_{24} + 6O_2 \rightarrow 12CO + 12H_2$ | 2.312E7 | 1 | 1.965E4 | $p^{0.3}[C_{12}H_{24}]^{0.5}[O_2]$ | This work |
| <i>Wet-CO mechanism</i> | | | | | |
| $H_2 + O_2 = OH + OH$ | 1.700E13 | 0 | 2.407E4 | Standard | 16,17 |
| $OH + H_2 = H_2O + H$ | 2.190E13 | 0 | 2.590E3 | Standard | 16,17 |
| $OH + OH = O + H_2O$ | 6.023E12 | 0 | 5.500E2 | Standard | 16,17 |
| $O + H_2 = H + OH$ | 1.800E10 | 1.0 | 4.480E3 | Standard | 16,17 |
| $H + O_2 = O + OH$ | 1.220E17 | -0.91 | 8.369E3 | Standard | 16,17 |
| $M + O + H = OH + M$ | 1.000E16 | 0 | 0 | Standard | 16,17 |
| $M + O + O = O_2 + M$ | 2.550E18 | -1.0 | 5.939E4 | Standard | 16,17 |
| $M + H + H = H_2 + M$ | 5.000E15 | 0 | 0 | Standard | 16,17 |
| $M + H + OH = H_2O + M$ | 8.400E21 | -2.0 | 0 | Standard | 16,17 |
| $CO + OH = H + CO_2$ | 4.000E12 | 0 | 4.030E3 | Standard | 16,17 |
| $CO + O_2 = CO_2 + O$ | 3.000E12 | 0 | 2.500E4 | Standard | 16,17 |
| $CO + O + M = CO_2 + M$ | 6.000E13 | 0 | 0 | Standard | 16,17 |
| <i>Soot formation global step</i> | | | | | |
| $C_{12}H_{24} \rightarrow 12C_s + 12H_2$ | 4.4947E15 | -1.94 | 1.610E4 | $[C_{12}H_{24}]^{1.81}[O_2]^{-0.5}$ | This work |
| <i>Heterogeneous soot oxidation</i> | | | | | |
| $C_s + 0.5O_2 \rightarrow CO$ | 1.0 | 0. | 0. | $72R_{ox}[C_s]/(\rho_s D_s)$ | This work 23 |
| $R_{ox} = K_A p_{O_2} \chi / (1 + K_Z p_{O_2})$ $+ K_B p_{O_2} (1 - \chi)$ $\chi = 1 / (1 + (K_T / K_B) p_{O_2})$ | | | | | |
| K_A | 2.0000E1 | 0 | 1.5098E4 | — | — |
| K_B | 4.4600E-3 | 0 | 7.6497E3 | — | — |
| K_T | 1.5100E5 | 0 | 4.8817E4 | — | — |
| K_Z | 2.1300E1 | 0 | -2.063E3 | — | — |
| <i>Homogeneous soot oxidation</i> | | | | | |
| $C_s + OH = CO + H$ | 1.2200E9 | 0.5 | 0 | Standard | This work |

^aM is third-body collision partner and $K = AT^B \exp(-E/RT)$.

soot slowly. This is because paraffins have to be broken up into smaller fragments first, from which fusing of the fragments occurs to form naphthenes and aromatics, and PAHs form eventually and indirectly (fragmentation-polymerization).^{19,20} These PAHs then undergo a series of physical processes to form coagulated soot particles. Frenklach et al.²¹ developed a comprehensive soot formation mechanism in which 180 species and 619 elementary reactions are used in an attempt to describe the aforementioned soot formation processes. However, at the present moment, it is far too expensive to be incorporated into a CFD code while the oxidation of those 180 species was not even considered. It is anticipated that the number of species and elementary reactions will be more than doubled if the oxidation of those 180 intermediate species is attempted. Nickerson and Johnson⁹ abridged the Frenklach et al.²¹ model to 19 reactions. However, their model⁹ completely ignores the fast condensation-polymerization process, and a soot formation mechanism of 19 reactions is still of considerable size. A global step that makes soot directly from $C_{12}H_{24}$ is used instead, as shown in Table 3. For convenience, pseudo-gas graphite carbon C_s is used to represent soot.

The formulation of the soot formation global step follows that of a previous study²² where the soot formation is assumed to be a function of temperature and oxygen and soot building block concentrations. The soot building block was taken to be acetylene,²⁰ expressed as C_2 hydrocarbons. The global rates were determined by direct comparison of the quasi-global model (with soot formation global step and heterogeneous soot oxidation step) predictions, using Exxon jet-stirred combustor data²² for neat fuels toluene and *iso*-octane. The effect of species radiation was measured as a heat loss and included in the jet-stirred combustor modeling. Notice the equivalent number of C_2 hydrocarbons for neat fuel toluene is three and one-half, whereas that for *iso*-octane is five. In this study, the equivalent number of C_2 hydrocarbons for surrogate fuel $C_{12}H_{24}$ is six. The preexponential factor is thereby adjusted slightly to account for the effect of increase in equivalent number of C_2 hydrocarbons.

Exxon's jet-stirred combustor data²² for neat fuels, with which the soot formation global step was established, indicated signifi-

cant soot emissions from toluene combustion and negligible soot emissions from *iso*-octane combustion. The fuel concentration in the soot formation step is, therefore, essentially all cyclic hydrocarbons. This is reasonable because the condensation-polymerization is much faster and greater than that of fragmentation-polymerization as soot formation mechanism. This model was further tested with jet-stirred combustor data¹⁷ using toluene and *iso*-octane fuel blends (78.5/12.5 and 62.5/37.5) and the model-predicted soot emissions agreed very well with those of the data. Hence, it can be reasonably assumed that the effects of both routes are lumped into the global step until new data are available.

Jet-stirred combustor data characterizes the accuracy of the heat release and postflame species concentrations of the kinetics mechanism. The generality of the quasi-global kinetics model was tested by considering other experiments characterizing different aspects of the combustion mechanism. Initiation processes, as measured with shock-tube experiments, were considered as a severe test of the model that was developed with jet-stirred combustor data that are controlled primarily by recombination reactions that occur during the latter stages of combustion. Model predictions were compared with shock tube and flow reactor ignition delay times data.¹⁷ The agreements were excellent for both toluene and *iso*-octane neat fuels. Another severe test for the model is the stability behavior, as measured with jet-stirred combustor blowoff limits, which is controlled by the flow residence time. Model predictions were compared with jet-stirred combustor loading parameter data.¹⁷ Again, the comparisons were excellent.

Heterogeneous Soot Oxidation

The rates of carbon oxidation were first measured and fitted with a heterogeneous reaction model involving three elementary steps and two active carbon sites to form CO (Ref. 23). These rates were adopted by several investigators as the rates for heterogeneous soot oxidation. For example, earlier studies^{17,22} used a one-step equation that oxidizes soot with molecular oxygen to form CO_2 , whereas

the reaction rates are those of Ref. 23, but the rate expression was modified slightly. In 1995, Hier²⁴ reported that Roth et al.²⁵ and Olander et al.²⁶ independently confirmed that the reaction forming CO is much more likely than that forming CO₂. Roth et al.²⁵ used laser absorption to confirm the presence of CO and the absence of CO₂, whereas Olander et al.²⁶ used mass spectrometry to determine that the reaction forming CO was at least two orders of magnitude more probable than that forming CO₂. Based on those assertions, this study simplifies the three-step reactions²³ to a one-step global kinetics forming CO, while maintaining the original rates and the heterogeneous rate expression form,²² as shown in Table 3. Notice a nominal soot density of 2 g/cm³ and a nominal soot particle diameter of 250×10^{-8} cm are used in the rate expression.

Homogeneous Soot Oxidation

Not only is the OH radical an important controlling species of the heat release in combustion processes, as noted by one of the major premises of the quasi-global kinetics, but there is also evidence that OH dependent oxidation of the soot needs to be considered under many flame conditions, especially in hydrocarbon fueled exhaust plumes.^{27,28} The OH-dependent homogeneous soot oxidation reaction from Slack et al.²⁷ is, therefore, included in the present kinetics model, as shown in Table 3. Notice this reaction is endothermic, whereas the heterogeneous soot oxidation reaction is exothermic. Also, instead of the irreversible reaction in its original form,²⁷ a reversible reaction is used because it produces better results with the following validation cases. Finally, all of the chemical reactions are solved simultaneously and coupled with the transport equations during design calculations. That is, different reaction or reactions may take precedence over others at various stages of the combustion processes or under various flow and thermal environments. For example, it is found in the following benchmark studies that the homogeneous soot oxidation is invoked mostly in the exhaust plume regime.

Application to Kerosene-Fueled Thrust Chambers

Pennsylvania State University (PSU) Tripropellant Combustor

The maximum combustion chamber pressure achievable is usually associated with the combustion efficiency. The proposed thermophysics model is incorporated with a CFD code, FDNS,^{29,30} to compute the chamber pressure of an unelement shear triaxial tripropellant combustor.³¹ The test rig is comprised of several sections, including an injector assembly, igniter, window, blank sections, and a nozzle assembly. Liquid RP-1 (LRP) is introduced through the central post of the triaxial tri-propellant injector and swirled using a tangential swirl nut, whereas gaseous H₂ (GH₂) and gaseous O₂ (GO₂) are injected through the first and second (outer) annuluses, respectively. Details of the injector and the thrust chamber setup may be found in Refs. 15 and 31, whereas the chamber operating conditions used for model validation may be found in Ref. 31.

FDNS is a multidimensional, multispecies, viscous flow, and pressure-based reacting flow solver. It was developed at Marshall Space Flight Center (MSFC) and is continuously being improved by MSFC personnel and its supporting contractors. When the proposed thermophysics formulation of kerosene combustion is incorporated and validated with a flow solver like FDNS, realistic performance computations can be performed to support the design of kerosene-fueled injectors and thrust chambers, rather than relying on one-dimensional type of system performance calculations. FDNS solves simultaneous liquid droplets-gas dynamics by combining the volume-of-fluid (VOF) and Eulerian/Lagrangian tracking methods into a unified algorithm for efficient calculation of multiphase flows at all speeds. The gas-liquid interface mass, momentum, and energy conservation properties are modeled by continuum surface mechanisms. Details of the solution procedure for liquid droplets-gas governing equations may be found in Refs. 30 and 32. In the VOF formulation, the weight-averaged conservation equations of mass, momentum, and scalar variables are formulated in an Eulerian framework. Current formulation considers the vaporization of liquid droplets into gases, but not the direct vaporization of liquid

jet core into gases. An empirical mass stripping rate is applied to the VOF equation along the liquid-gas interface for liquid intact core resolution. The stripped liquid mass undergoes secondary breakup process to form smaller droplets. The Lagrangian particle tracking method is used to treat the dynamics and heat/mass transfer of droplets as statistical computational parcels. Energy and momentum are solved for each parcel for every species, and relative enthalpy is the dependent variable for the droplet energy equation. For simplicity, parcel temperature is assumed to be constant at any time instant, but varies throughout its life expectancy via local heat transfer at the surface and vaporization. The heat capacity and latent heat of vaporization for liquid droplets are taken from Ref. 12.

An axisymmetric thrust chamber is formulated, and the computational domain covers the entire thrust chamber. As such, there is no ambiguity in the exit flow boundary condition once the throat flow is choked. For comparison purpose, a gaseous RP-1 (GRP)/GH₂/GO₂ injector flowfield is computed first. After its convergence, the GRP flow inlet is then replaced with the LRP flow inlet, and an LRP/GH₂/GO₂ injector flowfield computation is begun. To start the calculation, a cold-flow thruster flowfield is computed first until the nozzle flow at the end of the combustor choked. The propellants in the mixing layers are then ignited by temporarily imposing a hot spot with an elevated temperature (1000 K) in the flowfield. Once ignited, the flame propagates upstream and spreads downstream, where the location or the added energy of the temporary hot spot does not influence the final solution. Because of the backward-facing step formation created by the injector faceplate and the sidewall, a flow recirculation forms to serve as a flame holder. A fixed mass flow rate boundary condition is imposed at the flow inlet, and the inlet total enthalpy is conserved. The flow properties at the nozzle exit plane are extrapolated from those of the interior.

Figure 3 shows the computed scalar contours for the unelement GRP/GH₂/GO₂ injector/combustor. Because the LRP jet is replaced with the GRP jet, there are no α_{LRP} contours. The first three scalar contours are those of the reactants GRP, GH₂, and GO₂. The mixing layers among GRP, GH₂, and GO₂ can be seen from those three contours. The pressure contours show a nearly constant pressure inside the combustion chamber, which is expected because the propellant

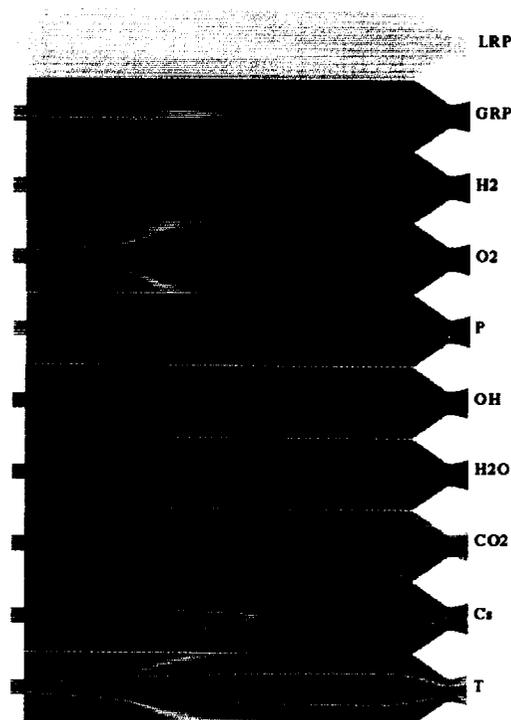


Fig. 3 Computed scalar contours for a unelement GRP/GH₂/GO₂ injector/combustor: α_{LRP} , 0–1; α_{GRP} , 0–1; α_{H_2} , 0–1; α_{O_2} , 0–1; P , 4.7–34.2; α_{OH} , 0–0.12; α_{H_2O} , 0–0.87; α_{CO_2} , 0–0.39; α_{Cs} , 0–0.17; and T , 251–3528.

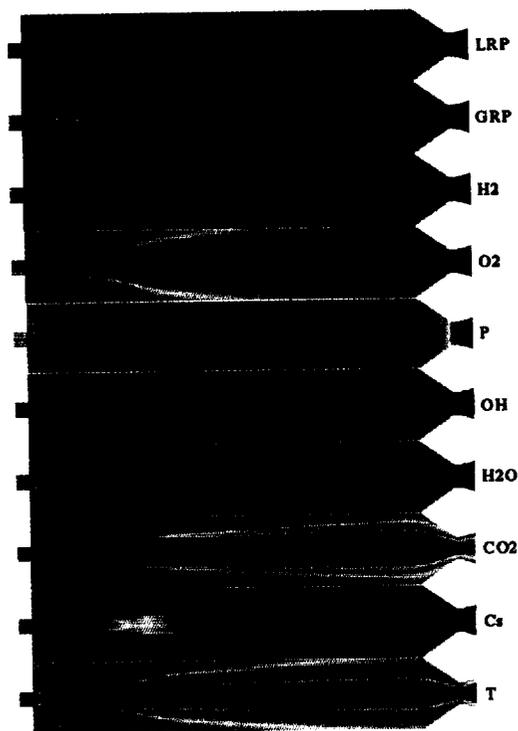


Fig. 4 Computed scalar contours for a unielement LRP/GH₂/GO₂ injector/comburntor: α_{LRP} , 0–1; α_{GRP} , 0–1; α_{H_2} , 0–1; α_{O_2} , 0–1; P , 4.7–34.2; α_{OH} , 0–0.12; α_{H_2O} , 0–0.87; α_{CO_2} , 0–0.39; α_{Cs} , 0–0.17; and T , 251–3528.

jet speeds are subsonic. The next three contours show the mass fractions of the three major combustion products: OH, H₂O, and CO₂. The high-concentration regions represent the flame front. Following those three scalar contours are the C_s mass fraction contours in which the incipient soot formation starts at the initial mixing layer. Most of the soot in the flame zone and nozzle is burned off by the heterogeneous and homogeneous oxidation reactions. Then there are the temperature contours, and again the high temperature region represents the flame front. The close association of high OH concentration with high temperature emphasizes the importance of OH in initiating and sustaining the combustion.

Figure 4 shows the computed scalar contours for the unielement LRP/GH₂/GO₂ thrust chamber. The first contours show the LRP jet core and the subsequent trajectories and sizes of the droplets stripping from the liquid jet. It can be seen that the droplets stripped off from the liquid jet core move downstream along the centerline for a short distance. The droplets then expand along with the gaseous jet. None of the droplets appears to survive past the flame front and a short distance into the convergent section. Most of the surviving droplets appear near the flame front and inside the GRP core, while a small amount of bigger droplets appears close to the centerline and creates an appearance of a hole near the centerline of the spray. The hole phenomenon can be traced to the swirling motion of the LRP jet, through a tangential swirl nut situated upstream of the injector.³¹ Secondary reasons include the droplet stripping and breakup mechanism. For example, it is known from test observations that bigger droplets often appear near the centerline. The mass stripping model, therefore, assumes a droplet size distribution along the liquid jet core surface with the biggest droplet stripped from the tip. Because the stripping rate is assumed to be uniform along the jet core surface, the droplet number density is a minimum at the tip. Notice the swirling smaller droplets expand laterally easier with the expanding gas and are heated up sooner. That leads to a lower surface tension because of a higher droplet temperature. That in turn leads to a higher Weber number and a higher secondary breakup rate. The result is an appearance of more droplets away from the centerline. On the other hand, the bigger droplets stripped off from the tip of the jet core that move along the centerline are bathed in

Table 4 Comparison of chamber pressures

| Model and test | P_c , atm |
|--------------------------------------|-------------|
| Test data | 34.2 |
| GRP/GH ₂ /GO ₂ | 35.8 |
| LRP/GH ₂ /GO ₂ | 33.5 |

a colder gas core with less chance of secondary breakup, thereby the appearance of fewer droplets. In addition, any droplet trajectory that falls a small distance near the centerline is reflected off due to the symmetry boundary condition. Hence, although the effects of the droplet entering the centerline cells, such as drag force and heat transfer, are retained, the new location of the reflected droplet is off centerline, which again leads to an appearance of fewer droplets. Note that the initial angle of the droplets stripping off along the liquid jet core surface is randomly selected.

The rest of the scalar contours resemble those of Fig. 3 qualitatively, with some differences caused by the modeling of the liquid jet and droplets. For example, the length of the GRP jet in Fig. 4 appears to be longer than that in Fig. 3, due to the added delay of atomization and vaporization processes. The overall temperature in Fig. 4 appears lower than that in Fig. 3, possibly caused by the latent heat loss of vaporizing liquid droplets. As such, the computed chamber pressure of the LRP/GH₂/GO₂ thruster is slightly lower than that of the GRP/GH₂/GO₂ thruster. Again, the chamber pressure is nearly constant. In addition, the overall computed soot concentration appears to be lower in the LRP/GH₂/GO₂ thruster.

Table 4 shows the comparison of computed chamber pressures with that of the test. It can be seen that the computed chamber pressures from both models compare reasonably well with that of the measurement, although it is anticipated that the GRP/GH₂/GO₂ model-predicted chamber pressure would be slightly higher. On the other hand, the demand for computational resources is higher, and empirical values for such parameters as the stripping rate and droplet size distribution have to be determined for the multiphase flow solution.

Because the latent heat decreases as chamber pressure increases, it is postulated that the states of liquid and gas may be indistinguishable under high-pressure rocket chamber environments. That postulation seems to agree with an experimental observation,³³ a faster rate of gasification is associated with elevated chamber pressures, of the combustion time for an RP-1 droplet. As such, the solution from the gaseous-phase model is probably as good as that of the multiphase flow model, but with a lesser demand for computational resources. The reasonable agreement of the chamber pressures in Table 4 is, therefore, attributed to the proposed thermophysics characterization rather than the choice of a single-phase or a multiphase flow option.

NASA MSFC 40,000-lb Thruster Plume Radiation

The proposed thermophysics model is also incorporated with the FDNS code for computing and comparing the predicted radiative heat fluxes with those of a test for kerosene-fueled thruster plume. The radiometers of the test are located downstream of the thruster exit plane and the lines of sight are perpendicular to the plume centerline. Figure 5 shows typical computed scalar contours for temperature, CO₂, H₂O, and C_s mass fractions. The four vertical lines across the plume indicate the lines of sight of the radiation measurement where the first vertical line from the nozzle exit plane is designated as the line of sight of radiometer R₁, and so on. The line of sight of radiometer R₂ is closest to the computed plume Mach disk. The flow model is an axisymmetric formulation, and the computational domain is five times longer than shown to include enough plumes for the wide-angle radiation calculations. Details of injection layout in the combustor such as the multiple fuel and oxidizer injection ports, a central fuel jet, and a wall film coolant jet are included in the computation. The scalar contours in Fig. 5 show striations of these jets converging near the throat, expanding in the nozzle and thrusting into the atmosphere. The interaction of the exhaust plume with the initially quiescent air creates an eddy-like mixing layer in which the remaining reactants afterburn. This is

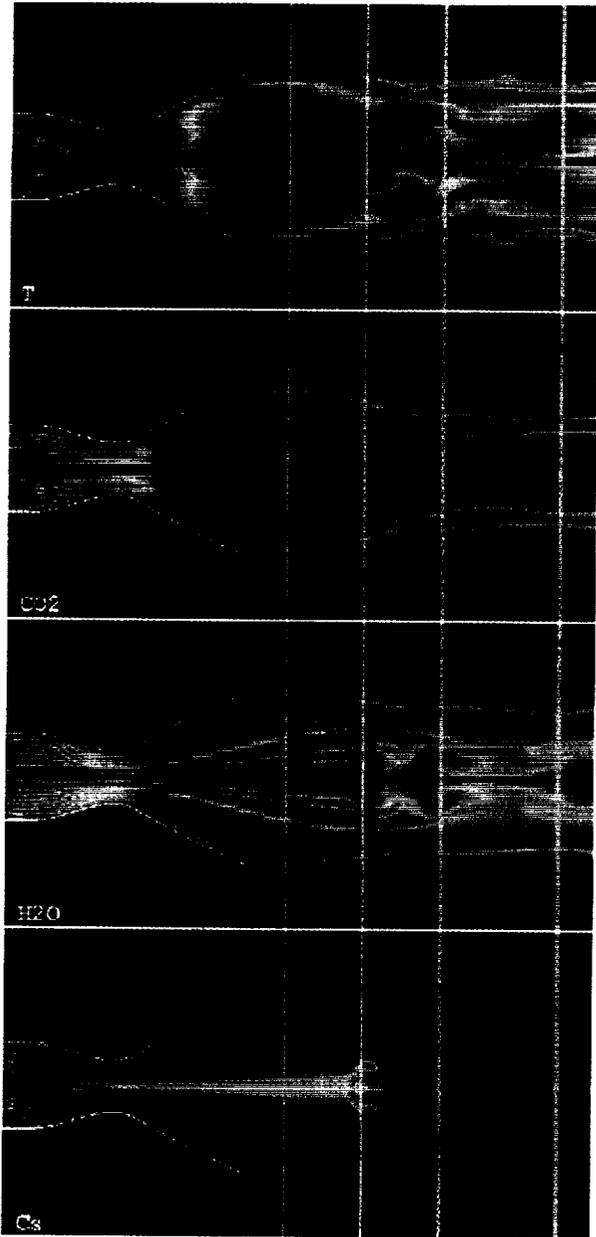


Fig. 5 Computed scalar contours for a kerosene fueled thruster and plume: T , 93–3045; α_{CO_2} , 0–0.5; $\alpha_{\text{H}_2\text{O}}$, 0–0.3; and α_{C_s} , 0–0.3.

shown in the plume–air mixing region of the temperature contours in Fig. 5. The film coolant essentially forms a protective, sooty layer along the thruster wall and mixes into the free shear layer, as shown in the C_s contours. Also shown in the C_s contours is a central soot core resulting from the central fuel jet injection. The triple shocks (lip shock, Mach disk, and reflect shock) are clearly seen in the temperature contours. Overall, the computed thermoflowfield appears to be reasonable. These scalar contours are plotted because CO_2 , H_2O , and C_s are major radiators of a kerosene-fueled thruster plume. The local concentrations of these radiators and temperature decide the strength of the radiation.

Parametric studies are performed to study the effect of homogeneous soot oxidation on the radiation signals. Table 5 shows the comparison of computed plume radiation with that of the test. The plume radiation is computed with a GASRAD radiation code³⁴ with which extensive benchmarks for rocket plumes have been performed. The radiation model is a statistical band model for exponential line strength distribution with Lorentz/Doppler line shapes for gaseous species and an approximate treatment of carbon particles. Details of the GASRAD radiation formulations may be found in Ref.

Table 5 Comparison of computed plume radiation with that of the test

| Model and test | R_1 | R_2 | R_3 | R_4 |
|-----------------------------------|-------|---------|-------|-------|
| θ | 4 | 180 | 4 | 5.5 |
| Q , test data | 10–12 | 5.4–6.0 | 75–95 | >70 |
| Q , without soot oxidation | 120.7 | 2.9 | 55.7 | 34.0 |
| Q , irreversible soot oxidation | 8.4 | 1.9 | 26.5 | 25.4 |
| Q , reversible soot oxidation | 14.1 | 5.4 | 131.9 | 117.3 |

34. Note that the hot firing of a rocket thruster is transient in nature and that the radiation signals are taken when the chamber pressure reaches an approximate constant. As a result, the plume boundary layer is unsteady, and the usefulness of the radiation measurement often depends on the view angle of the radiometer. Among the four radiometers, only radiometer R_2 has a wide-angle view (180 deg) and is least likely to be influenced by the unsteady motion of the free shear layer. On the other hand, the measurements from other three radiometers are of the narrow-angle category and, therefore, are susceptible to the unsteady plume motion. Note from posttest examination that there was some shrinkage of the throat due to soot accumulation, resulting in some slight drifting of the chamber pressure.

From Table 5, the thermophysics model using the reversible homogeneous soot oxidation reaction produces the best comparison with the wide-angle data and reasonable comparison with those of the narrow-angle measurements (two out of three). The overprediction at R_3 is attributed to the combination of the narrow view angle and the unsteadiness of the free shear layer. On the other hand, when the original irreversible form of the homogeneous soot oxidation reaction is used, soot burns off quickly, and all of the radiations are underpredicted. Without the homogeneous soot oxidation, the model overpredicts at radiometer R_1 , whereas it underpredicts at radiometers R_2 , R_3 , and R_4 . The reversible homogeneous soot oxidation reaction is, therefore, selected.

In summary, the proposed thermophysics characterization of kerosene combustion is demonstrated with two rocket engine applications. The combustion physics covered in the combustion efficiency benchmark of the PSU tripropellant combustor include initiation, flame propagation, heat release, flame holding, mixing, multiphase flow, and droplet vaporization; the combustion physics covered in the NASA MSFC 40,000-lb thruster plume radiation benchmark include air entrainment, mixing, afterburning, radiation, and shock formation. However, note that as the computer storage and speed increase with the advances in computational technology, alternative approaches aiming toward more detailed schemes may be devised. In addition, caution should be made when applying the proposed models beyond its range of validity. Nevertheless, this study offers an anchored and cost-effective model for incorporation with standard CFD codes for design calculations. The rationale given provides a systematic approach for model improvement when new data are available.

Conclusions

A thermophysics characterization of kerosene combustion is developed for incorporation with advanced CFD methodologies for kerosene-fueled rocket engine design calculations. The computational efficient model consists of a surrogate fuel model representing kerosene/RP-1 fuels, a thermodynamics model anchored with the heat of combustion, and a quasi-global kinetics model describing the combustion processes, including the soot formation and oxidation reactions. The rationale of the modeling approach is given. The benchmark results indicate that the proposed thermophysics model can be used to support the kerosene-fueled thrust chamber design applications and plume definitions.

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